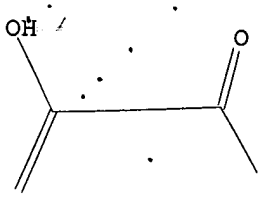
```
     (FILE 'HOME' ENTERED AT 15:05:23 ON 18 NOV 2003)

     FILE 'CAPLUS' ENTERED AT 15:05:32 ON 18 NOV 2003
L1                STRUCTURE UPLOADED
                  S L1

     FILE 'REGISTRY' ENTERED AT 15:06:32 ON 18 NOV 2003
L2              4 S L1

     FILE 'CAPLUS' ENTERED AT 15:06:32 ON 18 NOV 2003
L3              4 S L2
                  S L1

     FILE 'REGISTRY' ENTERED AT 15:06:41 ON 18 NOV 2003
L4            200 S L1 FULL

     FILE 'CAPLUS' ENTERED AT 15:06:42 ON 18 NOV 2003
L5            468 S L4 FULL
L6              0 S L5 AND ELECTROPHILIC GROUP
L7             57 S L5 AND OXIDIZ?
L8              7 S L7 AND COMPLEX
L9              6 S L7 AND COMPLEX AND (O OR S OR N OR SE OR P)
L10               STRUCTURE UPLOADED
L11          2499 S L0
                  S L10 AND COMPLEX AND (O OR S OR N OR SE OR P)

     FILE 'REGISTRY' ENTERED AT 15:14:53 ON 18 NOV 2003
L12             4 S L10

     FILE 'CAPLUS' ENTERED AT 15:14:54 ON 18 NOV 2003
L13             3 S L12
L14             0 S L13 AND COMPLEX AND (O OR S OR N OR SE OR P)
L15            51 S L11 AND COMPLEX AND (O OR S OR N OR SE OR P)
L16             1 S L15 AND OXIDIZ?
L17               STRUCTURE UPLOADED
                  S L17

     FILE 'REGISTRY' ENTERED AT 15:18:35 ON 18 NOV 2003
L18             5 S L17

     FILE 'CAPLUS' ENTERED AT 15:18:36 ON 18 NOV 2003
L19             5 S L18
                  S L17

     FILE 'REGISTRY' ENTERED AT 15:18:43 ON 18 NOV 2003
L20           256 S L17 FULL

     FILE 'CAPLUS' ENTERED AT 15:18:44 ON 18 NOV 2003
L21           497 S L20 FULL
L22            26 S L21 AND COMPLEX AND (O OR S OR N OR SE OR P)
L23             6 S L22 AND OXIDIZ?

=> s l15 and oxidiz?
        363752 OXIDIZ?
L24             1 L15 AND OXIDIZ?

=> s l15 and electrophilic group
         22314 ELECTROPHILIC
       1340369 GROUP
           188 ELECTROPHILIC GROUP
                 (ELECTROPHILIC(W)GROUP)
L25             0 L15 AND ELECTROPHILIC GROUP

=>
```



Structure attributes must be viewed using STN Express query preparation.

```
=> s l0
L11       2499 L0

=> s l10 and complex and (O or s or n or se or p)
   REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.



SAMPLE SEARCH INITIATED 15:14:53 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   3314 TO ITERATE

 30.2% PROCESSED    1000 ITERATIONS                                 4 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:         62828 TO    69732
PROJECTED ANSWERS:               47 TO      483

L12            4 SEA SSS SAM L10



L13            3 L12


       1107803 COMPLEX
       1389029 O
       2493308 S
       2640024 N
        113418 SE
       2169529 P
L14            0 L13 AND COMPLEX AND (O OR S OR N OR SE OR P)

=> s l11 and complex and (O or s or n or se or p)
       1107803 COMPLEX
       1389029 O
       2493308 S
       2640024 N
        113418 SE
       2169529 P
L15           51 L11 AND COMPLEX AND (O OR S OR N OR SE OR P)

=> s l15 and oxidiz?
        363752 OXIDIZ?
L16            1 L15 AND OXIDIZ?

=> d ibib abs hitstr

L16  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         2000:367224  CAPLUS
```

DOGUMENT NUMBER: 133:114100
TITLE: Molecular and Electronic Structures of Bis(pyridine-2,6-diimine)metal Complexes [ML2](PF6) **n** (**n** = 0, 1, 2, 3; M = Mn, Fe, Co, Ni, Cu, Zn)
AUTHOR(S): De Bruin, Bas; Bill, Eckhard; Bothe, Eberhard; Weyhermueller, Thomas; Wieghardt, Karl
CORPORATE SOURCE: Max-Planck-Institut fuer Strahlenchemie, Muelheim an der Ruhr, D-45470, Germany
SOURCE: Inorganic Chemistry (2000), 39(13), 2936-2947
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

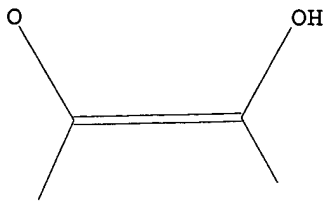
AB Mononuclear, octahedral first-row transition metal ion complexes mer-[MIIL02](PF6)2 contg. the tridentate neutral ligand 2,6-bis[1-(4-methoxyphenylimino)ethyl]pyridine (**L0**) and a MnII, FeII, CoII, NiII, CuII, or ZnII ion were synthesized and characterized by x-ray crystallog. Cyclic voltammetry and controlled potential coulometry show that each dication (except those of CuII and ZnII) can be reversibly 1-electron-**oxidized**, yielding the resp. trications [MIIIL02]3+, and in addn., they can be reversibly reduced to the corresponding monocations [ML2]+ and the neutral species [ML2]0 by two successive 1-electron processes. [MnL2]PF6 and [CoL2]PF6 were isolated and characterized by x-ray crystallog. Their electronic structures are described as [MnIIIL12]PF6 and [CoIL02]PF6 where (L1)1- represents the 1-electron-reduced radical form of **L0**. The electronic structures of the tri-, di-, and monocations and of the neutral species were elucidated in detail by a combination of spectroscopies: UV-visible, NMR, X-band EPR, Moessbauer, temp.-dependent magnetochem. Pyridine-2,6-diimine ligands are non-innocent ligands that can be coordinated to transition metal ions as neutral **L0** or, alternatively, as monoanionic radical (L1)1-. All trications are [MIIIL02]3+, and the dications are [MIIL02]2+. The monocations are described as [MnIIIL12]+ (**S** = 0), [FeIIL0L1]+ (**S** = 1/2), [CoIL02]+ (**S** = 1), [NiIL02]+ (**S** = 1/2), [CuIL02]+ (**S** = 0), [ZnIIL1L0]+ (**S** = 1/2) where the MnIII and FeII ions are low-spin-configurated. The neutral species are described as [MnIIL12]0, [FeIIL12]0, [CoIL0L1]0, [NiIL0L1]0, and [ZnIIL12]0; their electronic ground states were not detd.

REFERENCE COUNT: 51 THERE ARE 51 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=>
Uploading 181.str

L17 STRUCTURE UPLOADED

=> d l17
L17 HAS NO ANSWERS
L17 STR



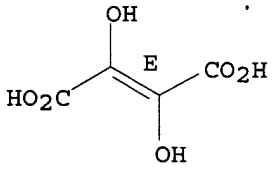
Structure attributes must be viewed using STN Express query preparation.

=> s l17
REG1stRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.

```
SAMPLE SEARCH INITIATED 15:18:36 FILE 'REGISTRY'
SAMPLE SCREEN SEARCH COMPLETED -   2124 TO ITERATE

 47.1% PROCESSED    1000 ITERATIONS                                  5 ANSWERS
INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS:  ONLINE  **COMPLETE**
                        BATCH   **COMPLETE**
PROJECTED ITERATIONS:        39716 TO    45244
PROJECTED ANSWERS:              17 TO      407

L18           5 SEA SSS SAM L17



L19           5 L18

=> s l17 full
   REGIstRY INITIATED
Substance data SEARCH and crossover from CAS REGISTRY in progress...
Use DISPLAY HITSTR (or FHITSTR) to directly view retrieved structures.




FULL SEARCH INITIATED 15:18:43 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -  41618 TO ITERATE

100.0% PROCESSED   41618 ITERATIONS                             256 ANSWERS
SEARCH TIME: 00.00.01

L20          256 SEA SSS FUL L17



L21          497 L20

=> s l21 and complex and (O or s or n or se or p)
       1107803 COMPLEX
       1389029 O
       2493308 S
       2640024 N
        113418 SE
       2169529 P
L22           26 L21 AND COMPLEX AND (O OR S OR N OR SE OR P)

=> s l22 and oxidiz?
        363752 OXIDIZ?
L23            6 L22 AND OXIDIZ?

=> d 1-6 ibib abs hitstr

L23  ANSWER 1 OF 6  CAPLUS  COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER:         1985:107657  CAPLUS
DOCUMENT NUMBER:          102:107657
TITLE:                    The production of hydroxyl radical from hydrogen
                          peroxide
AUTHOR(S):                Florence, T. M.
CORPORATE SOURCE:         Div. Energy Chem., CSIRO, Sutherland, 2232, Australia
SOURCE:                   Journal of Inorganic Biochemistry (1984), 22(4),
                          221-30
                          CODEN: JIBIDJ; ISSN: 0162-0134
```

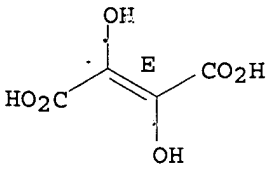
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The formation of OH.cntdot. from the oxidn. of GSH [70-18-8], ascorbic acid [50-81-7], NADPH [53-57-6], hydroquinone [123-31-9], catechol [120-80-9], and riboflavin [83-88-5] by H2O2 was studied using a range of enzymes and Cu and Fe complexes as possible catalysts. Cu-1,10-phenanthroline [15823-71-9] appeared to catalyze the prodn. of OH.cntdot. from H2O2 without superoxide radical being formed as an intermediate, and without the involvement of a catalyzed Haber-Weiss (Fenton) reaction. Superoxide radical was involved, however, in the Cu-catalyzed decompn. of H2O2, and in the oxidn. of GSH by **O**. For this latter oxidn., Cu-4,7-dimethyl-1,10-phenanthroline [23555-69-3] was a much more effective catalyst than the Cu **complex** of 1,10-phenanthroline, which is normally used. Mechanisms for these reactions are proposed, and the toxicol. significance of the ability of a variety of biol. reductants to provide a prolific source of OH.cntdot. when **oxidized** by H2O2 is discussed.
IT **133-38-0**
RL: BIOL (Biological study)
(hydroxy radical formation from hydrogen peroxide in relation to)
RN 133-38-0 CAPLUS
CN 2-Butenedioic acid, 2,3-dihydroxy-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L23 ANSWER 2 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1979:401485 CAPLUS
DOCUMENT NUMBER: 91:1485
TITLE: On the nature of biochemically generated hydroxyl radicals. Studies using the bleaching of **p** -nitrosodimethylaniline as a direct assay method
AUTHOR(S): Bors, Wolf; Michel, Christa; Saran, Manfred
CORPORATE SOURCE: Inst. Biol., Ges. Strahlen- Umweltforsch., Neuherberg, D-8042, Fed. Rep. Ger.
SOURCE: European Journal of Biochemistry (1979), 95(3), 621-7
CODEN: EJBCAI; ISSN: 0014-2956
DOCUMENT TYPE: Journal
LANGUAGE: English
AB An efficient scavenger for radiolytically generated hydroxyl (.bul.OH) radicals, **p**-nitrosodimethylaniline, was used to try to substantiate the presence of this **O** radical species in several biochem. systems. Most of the systems investigated had previously been assumed to generate .bul.OH radicals, e.g., the autoxidn. of 6-hydroxydopamine, the hydroxylating system NADH/phenazine methosulfate, and the oxidn. of xanthine or acetaldehyde by xanthine oxidase. No inhibition of the bleaching of **p**-nitrosodimethylaniline in oxygenated solns. by other scavengers of .bul.OH radicals was obsd. nor, in the case of xanthine/xanthine oxidase, by catalase and superoxide dismutase. Therefore, under biochem. conditions as opposed to radiolysis or photolysis, no freely diffusable .bul.OH radicals are formed. Rather, a strongly **oxidizing** .bul.OH-analogous **complex** probably represents the **p**-nitrosodimethylaniline-detectable species formed under these conditions.
IT **133-38-0**
RL: RCT (Reactant); RACT (Reactant or reagent)
(oxidn. of, hydroxyl radicals in)
RN 133-38-0 CAPLUS
CN 2-Butenedioic acid, 2,3-dihydroxy-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.

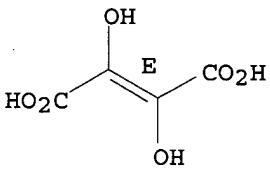


L23 ANSWER 3 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1966:422301 CAPLUS
DOCUMENT NUMBER: 65:22301
ORIGINAL REFERENCE NO.: 65:4185e-g
TITLE: Mechanism and model of peroxidase-oxidase reaction
AUTHOR(S): Yamazaki, I.; Yokota, K.; Nakajima, R.
CORPORATE SOURCE: Hokkaido Univ., Sapporo, Japan
SOURCE: Oxidases Related Redox Systems, Proc. Symp., Amherst, Mass., 1964 (1965), 1, 485-504, discussion 504-13
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Evidence is presented for several reaction paths for the free radicals formed from electron donor substrates by H2O2 reaction in the presence of peroxidase (I). Ascorbate oxidn. with H2O2 in the presence of I resulted in a const. concn. of semiquinone during several E.**S**.R. measurements. When dihydroxyfumarate (II) or triose reductone was treated similarly, the E.**S**.R. signals observed during the enzymic reactions disappeared completely when the reactions were over. In the presence of indoleacetic acid (III) and I, H2O2 induced formation of a ferroperoxidase **complex** (IV) with absorption max. at 423 m.mu.. When II was the electron donor, 1 mole of H2O2 was required to convert approx. 2 moles of I to IV. Hydroquinone and ferrocyanide were more effective in decompg. IV than were the corresponding **oxidized** forms, and anionic species were less active than cationic ones.

IT **133-38-0**, Fumaric acid, dihydroxy-
(oxidn. by peroxidase, radical formation in)
RN 133-38-0 CAPLUS
CN 2-Butenedioic acid, 2,3-dihydroxy-, (2E)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L23 ANSWER 4 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN
ACCESSION NUMBER: 1955:29964 CAPLUS
DOCUMENT NUMBER: 49:29964
ORIGINAL REFERENCE NO.: 49:5767h-i,5768a-b
TITLE: Oxidation-reduction processes taking part in the production of wine
AUTHOR(S): Rodopulo, A. K.
SOURCE: Vinodelie i Vinogradarstvo SSSR (1952), 12(No. 1), 21-4
CODEN: VIVSA6; ISSN: 0042-6318
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB cf. C.A. 48, 14102i. In the oxidation-reduction processes are involved the enzymes, polyphenol oxidase, ascorbic acid oxidase, cytochrome oxidase, peroxidase, catalase, and alc. dehydrogenase, and such systems as polyphenol .dblarw. quinones, ascorbic acid .dblarw. dehydroascorbic acid, EtOH .dblarw. AcH, reduced cytochrome c .dblarw. **oxidized** cytochrome c, coenzyme I .dblarw. dihydrocoenzyme I, and glutathione (RSH) .dblarw. RSSR. The biochem. conditions are discussed under which these

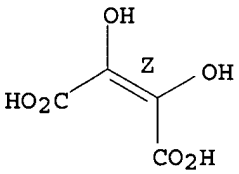
oxidation-reduction systems are present in must and wine. Bivalent iron (Fe++) also possesses biocatalytic properties. A canary-yellow **complex** salt (I) of Fe++ with tartaric acid, nearly insol. in water but sol. in dil. alk. solns., has been isolated; a mol. of H2O is strongly held on the I mol.: it cannot be removed even by treating I with H2SO4. During aging of wine I is pptd. in the containers. I shows a strong catalytic effect on the oxidation of tartaric acid (II) to dihydroxymaleic acid (III), which in turn, in the presence of atm. O is readily **oxidized** to dioxosuccinic acid (IV). Under aerobic conditions IV is further **oxidized** (with decarboxylation) to HO2CC(:O)CHO .fwdarw. C(:O)(CO2H)2 .fwdarw. HO2CCHO .fwdarw. (CO2H)2. This process is not desirable since the final products of this oxidation reaction affect the quality of wine. Under anaerobic conditions IV **oxidizes** II to III; this causes an accumulation of III in the wine. Ascorbic acid, if present, very rapidly **oxidizes** II to IV. To get a good-quality product the access of O to wine during the processing has to be regulated to keep the O concn. below 1 ml./l. wine.

IT **526-84-1**, Maleic acid, dihydroxy-
(formation and oxidation in musts and wines)

RN 526-84-1 CAPLUS

CN 2-Butenedioic acid, 2,3-dihydroxy-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L23 ANSWER 5 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1930:11597 CAPLUS

DOCUMENT NUMBER: 24:11597

ORIGINAL REFERENCE NO.: 24:1271b-f

TITLE: Mechanism of oxidation processes. XVIII. Further experiments on the activation of hydrogen peroxide by iron

AUTHOR(S): Wieland, Heinrich; Franke, Wilhelm

SOURCE: Ann. (1929), 475, 1-19

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 23, 4918. The **oxidizing** action of H2O2 on NaAsO2, H3PO3 and NaH2PO2 in the presence of bivalent and tervalent Fe was studied with results similar to those previously observed with org. acids (C. A. 22, 1065). In the presence of Fe++ there is a primary oxidation impulse, after which the rate of oxidation is much the same whether Fe++ or Fe+++ is present. Variation of the concn. of H2O2 does not appreciably influence the primary effect until high concns. are reached, when a slight decrease of the primary oxidation impulse is seen. Cu++ salts have all inhibiting effect on the oxidation of H3PO2 in the presence of Fe++ salts. Cu+ salts have no activating action similar to Fe++ salts. It is probable, therefore, that the effect of the Cu++ salt is to **oxidize** the Fe++ salt to Fe+++ with the formation of a Cu+ salt. The influence of a change in the pH of the H3PO2 soln. was also studied. The primary oxidation at pH 0.6 was greater than at pH 7.0 but both were less than at pH 4.6. The presence of dihydroxymaleic acid (I) increases the activation by Fe++ salts and, at lower concns., the increase in effect is approx. proportional to the amt. added, but becomes much less as the concn. increases. This behavior is comparable with that observed in the activation of O by Fe++. Dihydroxytartaric acid (II) also catalyzes the activation by Fe++ salts but not to the same extent as I, so that activation by the latter cannot be attributed to the II formed. Thioglycolic acid also causes marked acceleration of the primary oxidation impulse. The action of H2O2 on linolenic acid, in the presence of Fe++ and Fe+++ salts, is similar to that observed for other org. acids. The

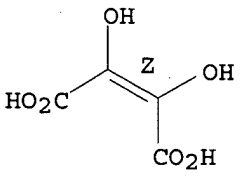
extent of activation obtained supports the conclusion that, contrary to the opinion of Manchot and Lehmann (C. A. 22, 2098), the effect is due not to the formation of a peroxide of Fe but to the formation of a **complex** between the Fe++ ion and the compd. to be **oxidized**. The latter becomes more readily **oxidizable**, while oxidation of the Fe is delayed. The extent of the primary oxidation impulse will depend on the rate of formation of this **complex**, its degree of dissocn. and the rate of oxidation of the acid in the **complex**.

IT **526-84-1**, Maleic acid, dihydroxy-
(effect on activation of H2O2 by Fe salts)

RN 526-84-1 CAPLUS

CN 2-Butenedioic acid, 2,3-dihydroxy-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



L23 ANSWER 6 OF 6 CAPLUS COPYRIGHT 2003 ACS on STN

ACCESSION NUMBER: 1928:36461 CAPLUS

DOCUMENT NUMBER: 22:36461

ORIGINAL REFERENCE NO.: 22:4320d-i,4321a-i,4322a-d

TITLE: Mechanism of oxidation processes. XIV. Activation of oxygen by iron

AUTHOR(S): Wieland, Heinrich; Franke, Wilhelm

CORPORATE SOURCE: Bayr. Akad. Wissenschaften zu Munchen

SOURCE: Ann. (1928), 464, 101-226

DOCUMENT TYPE: Journal

LANGUAGE: Unavailable

AB cf. C. A. 22, 2574. The autoxidation of solns. of ferrous salts has been studied with AcONa and AcOH as a buffer. Absorption of O follows the unimol. law. The temp. coeff. of the process is normal, while a change from pH 5 to 7 accelerates the reaction 4 or 5 times. At pH 5, neutral salts have little effect on the rate of autoxidation, although Na2SO4, possibly because it produces **complex** salts, causes diminution of the reaction velocity to 0.5 its previous value. The rate of autoxidation of slightly hydrated FeCl3 is greater in Me2CO than in EtOH or iso-PrOH, greater in these solvents than in MeOH and least in H2O. The autoxidation of a no. of acids in the presence of Fe salts has been studied. In general FeSO4 is the added Fe salt and an acetate buffer is used. Formic acid. Autoxidation of the ferrous salt induces autoxidation of formate, the latter ceasing when no more ferrous salt remains, since ferric Fe does not **oxidize** HCO2H. Lactic acid. Autoxidation of the lactate is more rapid than that of the formate, about 1/8 of the O absorbed by the system during the complete oxidation of the Fe being used to **oxidize** the lactate to CO2, AcH and (some) pyruvic acid. Autoxidation is most rapid at pH 8.0 and is slower in air than in pure O. Pyruvic acid. This case is very similar to that of lactic acid: in neither case does ferric Fe **oxidize** the acid. Tartaric acid. This autoxidation is investigated very fully. Small changes in conditions very greatly affect the progress of the reaction. Ferric salts do not initiate autoxidation of tartaric acid but play a considerable part in the autoxidation of the acid in the presence of ferrous salts, since the dihydroxymaleic acid (I) formed is **oxidized** by ferric, producing ferrous salts. The autoxidation proceeds much further in acid than in neutral solns. and has a normal temp. coeff. up to 20.degree.. At 30.degree., however, the process is not appreciably quicker than at 20.degree.. To some extent, the process is catalytic in nature, because of the reduction of ferric salts by the I formed. I acts as a strong positive catalyst for a similar reason. The autoxidation process is greatly accelerated by Na2SO4 and somewhat accelerated by NaNO3 or by CuSO4, while NaCl, NaI and NaBr act as strong retardants. p-C6H4O2 also has a retarding effect. Increased

pressure of O accelerates autoxidation, but the total amt. of O used is less than is the case with lower pressures. Dihydroxymaleic acid. Because of the slight soly. of the K and Na salts of I, buffering is best effected by AcOH and AcOLi. The spontaneous decompn. of a buffered soln. (pH 4.8) of I (atm. of N) is markedly affected by ferrous salts. Substitution of phthalate for acetate as a buffer has only a slight effect. Phosphate produces marked retardation and addn. of pyrophosphate in addn. further retards the velocity of autoxidation. Buffering with glycine causes acceleration. At pH 1.4 and 13, autoxidation is markedly slower than at intermediate acidities, pH 5 being the optimum condition. The spontaneous autoxidation of I in the absence of Fe proceeds more rapidly in alk. than in acid soln. The main reaction involved is I + 1/2 O2 .fwdarw. HO2CCOCOCO2H. Ferric salts **oxidize** I (pH 5, AcOH and AcOLi) to diketosuccinic acid, which, during the autoxidation process, gives (CO2H)2 and mesoxalic acid in the ratio of 1:2, the latter slowly giving (CO2H)2. Glyceric acid. This case is similar to tartaric acid. Added ferrous salt produces an effect roughly proportional to its concn. Thioglycolic acid. Cu salts are in general more positively catalytic of the autoxidation of this acid than are those of Fe, but the latter become more effective in the neighborhood of the neutral point. H2SO4 is a product of autoxidation, which is retarded by cyanides. Hydroquinone. The oxidation of this compd. by ferric salts renders the autoxidation of hydroquinone in the presence of ferrous salts similar to that of I. The velocity of change depends very largely on the pH. Near the neutral point, ferrous salts reduce p-C6H4O2 so that the basis of the autoxidation process is HOC6H4OH + 2Fe... .dblarw. O:C6H4:O + 2Fe.. + 2H.. The buffer used may have a considerable effect on the mobility of the equil. Thus, autoxidation is particularly facile in the presence of a AcONa buffer, less so with Na glycerate and much less so with Na phthalate. The catalytic action of Fe salts in this process has its optimum within certain fairly narrow limits of concn. p-C6H4O2 has a marked retarding effect on the autoxidation of hydroquinone, probably owing to the formation of an inactive Fe-quinhydrone **complex**. It is difficult to recognize the mechanism of the autoxidation as one of true catalysis and it may be that ferric salt is the effective oxidant of the hydroquinone. This would explain why in the slow autoxidation of hydroquinone that occurs in the absence of a buffer, ferrous and ferric salts produce effects of a similar magnitude. In buffered solns., ferrous Fe is more powerful in action than ferric, so that probably an O activation process is at work, in this case, on the part of a ferrous salt-acetate **complex**. Pyrocatechol. Here the accelerative influence of Fe in autoxidation is markedly stronger than with hydroquinone. Pyrogallol. This case is similar to pyrocatechol, but autoxidation is more rapid. The product is not purpurogallin but is the amorphous brown substance, resembling a humic acid, obtained in the H2O2-Fe oxidation of pyrogallol. K4Fe(CN)6 aids autoxidation but to a much smaller extent than simple Fe salts. Expts. have been carried out on the autoxidation of I in complete absence of Fe salts, to see if the known absorption of O by solns. of I is really due to the presence of unsuspected traces of Fe. While special purification of I (vacuum distn. in quartz) renders it more stable in this respect, Fe is not the initiator of the process but merely catalyzes a reaction in progress. This is supported by the fact that, in neutral solns. of the purified material, cyanide slightly accelerate autoxidation, whereas in the presence of traces of Fe, it markedly diminishes the acceleration due to the latter. Similar results have been obtained with hydroquinone. The autoxidation of hydroquinone itself produces H2O2 at pH 3.6, while when Fe is present no H2O2 is formed. Arsenious acid. According to Manchot (Z. anal. Chem. 27, 420(1901)) 1 equiv. of O is activated during the oxidation of Fe.. to Fe... and is used for the conversion of arsenite to arsenate. This is not actually realizable under all conditions of acidity. The most concd. weakly alk. soln. (pH 6) of arsenite obtainable shows an activation of only 0.88 equiv. For pH 10, corresponding with NaAsO2, activation corresponds to 0.6 equiv. and for more strongly alk. solns., corresponding with Na2HAsO3, it corresponds with not more than 1 equiv., in opposition to Gire's results (C. A. 14, 3027). When alky. corresponds to Na3AsO3, activation exceeds 1 equiv. of O, the extra (0.5 mol.) activation being due to

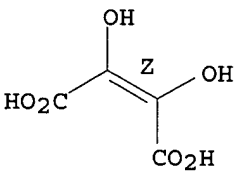
spontaneous autoxidation and not to oxidation of arsenite by ferric salts. Hypophosphorous acid. This acid is not appreciably **oxidized** by O in the absence of Fe salts. The autoxidation in the presence of Fe salts seems to be an induction effect, ceasing when all ferrous salt has become **oxidized**. It is little affected by pH. The results appear to show that the activation of mol. O by ferrous salts cannot be due to the intermediate formation of a peroxide, as suggested by Manchot. It is probable that the 1st stage in the autoxidation is the formation of a **complex** between the ferrous salt and the hypophosphite, rendering the H of the latter more active as regards oxidation. The 2nd stage is the very slow reaction 2Fe... + H3PO2 .fwdarw. H2O 2Fe.. + H3PO3 + 2H.degree.. H3PO3 behaves similarly to H3PO2 but the activation is less pronounced and is more influenced by the acidity conditions. Certain combined autoxidations have been studied. The autoxidation of H3PO2 in the presence of ferrous salts and I is catalytic in type, the pH of the soln. not greatly affecting the rate of change. Diketosuccinic acid (not tartaric or glyceric acid) behaves similarly to I but it is only slowly **oxidized** by ferric salt, whereas the latter is instantaneously **oxidized** by ferric salt in the presence of H3PO2. The mechanism of the combined autoxidation is discussed. Possibly a readily dehydrogenated ferric salt-diketosuccinic acid **complex** is formed as an intermediate. The autoxidation of HCO2H in the presence of ferrous salts is accelerated by I but the acceleration is less than in the above case of H3PO2. Diketosuccinic acid is again an active intermediate. Relatively large amts. of I are required to produce acceleration and the same is the case in the autoxidation of lactic acid in the presence of ferrous salts. I produces no acceleration of the autoxidation of hydroquinone-ferrous salts. The autoxidation of HCO2H-ferrous salt in the presence of thioglycolic acid is similar to the above case of HCO2H-I. The acid does not accelerate autoxidation until present in a certain concn. but after this is reached its effect is proportional to its concn. When lactic acid replaces HCO2H there is a more pronounced mutual activation, while when tartaric acid is used, less thioglycolic acid is required to accelerate the (more rapid) autoxidation. The autoxidation of H3PO2 and ferrous salts in the presence of thioglycolic acid is a case of true catalysis, due to the equil. between Fe...-thioglycolic acid and Fe..-dithiodiglycolic acid. This equil. must lie mostly on the Fe.. side, because of the marked initial activation which precedes the main, catalytic, stage. Activation is ascribed to the formation of a thioglycolic acid-ferrous salt **complex**. The autoxidation of H3PO2 in the presence of ferrous salts is not accelerated by pyruvic acid but the autoxidation of pyruvic acid in the presence of H3PO2 is markedly accelerated by traces of ferrous salts, giving a case of true catalysis. Some consideration is given to cases of direct addn. of O to an unsatd. linking, as distinguished from the above cases, in which H is removed from a substance. The autoxidation of linolenic acid and of lecithin is also discussed.

IT **526-84-1**, Maleic acid, dihydroxy-
(autoxidation of, in presence of Fe salts)

RN 526-84-1 CAPLUS

CN 2-Butenedioic acid, 2,3-dihydroxy-, (2Z)- (9CI) (CA INDEX NAME)

Double bond geometry as shown.



Sn^{+}, Hg^{+2}, Pt^{+2}

Lewis acid – BF_3, $AlCl_3$

=> d ibib abs hitstr

L2 ANSWER 1 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2001:380405 CAPLUS
DOCUMENT NUMBER: 135:9997
TITLE: Boron compounds and complexes as anti-inflammatory agents
INVENTOR(S): Miljkovic, Dusan
PATENT ASSIGNEE(S): Topgene, Inc., USA
SOURCE: PCT Int. Appl., 18 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2001035966	A1	20010525	WO 2000-US31354	20001114
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, CZ, DE, DE, DK, DK, DM, DZ, EE, EE, ES, FI, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
EP 1233772	A1	20020828	EP 2000-979177	20001114
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR				
JP 2003514023	T2	20030415	JP 2001-537958	20001114

PRIORITY APPLN. INFO.: US 1999-166938P P 19991119
WO 2000-US31354 W 20001114

AB Inflammation is affected by topical application of a boron contg. compd./complex in which a central tetrahedral boron atom is covalently bound to four ligands. At least one of the ligands preferably includes an oxygen, nitrogen, carbon, or sulfur atom, and preferably all four ligands include at least one such atom. Preferred ligands are saccharides and amino acids, including fructose, sorbitol, mannitol, xylitol, sorbose, serine and threonine. Esp. preferred ligands have a conformation with at least two hydroxyl groups, or one hydroxyl group and one amino group in a 1,2- and a 1,3- position relative to each other, providing a high assocn. const. in the range of about 3000 and about 20,000. The compds./complexes are preferably provided in formulations which provide good transdermal delivery, including appropriate solvent systems, microemulsions, and liposomes. Particularly targeted inflammations are those of the joints and skin, including burns such as sunburn. For example, liposomes contg. calcium **fructoborate** were prepd.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

=> d 2-4 ibib abs hitstr

L2 ANSWER 2 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 2000:433281 CAPLUS
DOCUMENT NUMBER: 133:63623
TITLE: Boron compounds and complexes as skin-rejuvenating agents
INVENTOR(S): Miljkovic, Dusan; Pietrzkowski, Zbigniew
PATENT ASSIGNEE(S): Topgene, Inc., USA
SOURCE: U.S., 13 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 6080425	A	20000627	US 1998-192814	19981116

PRIORITY APPLN. INFO.: US 1998-86826P P 19980526

AB Boron compds./complexes, other than boric acid and boric acid salts, are utilized for rejuvenating of skin. The compds./complexes have a central tetrahedral boron atom covalently bound to four ligands, which may be either identical or different from each other. Preferred ligands include an oxygen, nitrogen, carbon or sulfur atom, and more preferred ligands are saccharides or amino acids that form stable five- or six-membered rings with the boron atom. Esp. preferred compds. have a dissocn. const. of at least 3,000, and include a saccharide. Esp. preferred complexes include a sodium, potassium, magnesium or calcium cation. The compds./complexes are useful in rejuvenating skin, including decreasing skin wrinkles, improving skin thickness, increasing skin hydration, softness and elasticity, improving the skin color, and decreasing the no. and size of age spots. The compds./complexes are preferably provided in a suitable solvent system, a microemulsion or macroemulsion form, or a suitable liposome, and may be applied in any suitable form, including creams, bath salts, cosmetics, and shampoos. Phosphatidyl choline (0.250 g in 25 mL of chloroform) was evapd. at room temp. in vacuum with a rotary evaporator to provide a uniform transparent lipid film. Calcium fructo-borate (1 g in 50 mL) water was added at once to the lipid film. After shaking the mixt. for 2 h at 37.degree., and sonicating the mixt. for an addnl. 0.5 h at room temp., prepn. of the calcium fructo-borate liposome formulation was finished.

REFERENCE COUNT: 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 3 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN
ACCESSION NUMBER: 1998:682135 CAPLUS
DOCUMENT NUMBER: 129:301935
TITLE: Boron-carbohydrate complexes for use in nutrition
INVENTOR(S): Miljkovic, Dusan
PATENT ASSIGNEE(S): USA
SOURCE: PCT Int. Appl., 14 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9843652	A1	19981008	WO 1998-US6050	19980326
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
US 5962049	A	19991005	US 1998-45141	19980320
AU 9867800	A1	19981022	AU 1998-67800	19980326
EP 1001788	A1	20000524	EP 1998-913189	19980326
EP 1001788	B1	20030219		
R: BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, PT				
JP 2001518882	T2	20011016	JP 1998-541827	19980326
ES 2191291	T3	20030901	ES 1998-913189	19980326

PRIORITY APPLN. INFO.: US 1997-42883P P 19970331
US 1998-45141 A 19980320
WO 1998-US6050 W 19980326

AB Complexes of boron with sugars and/or sugar alcs. are utilized as nutritional supplements, with the carbohydrate portion being selected to provide a relatively high boron-sugar assocn. const. of .gtoreq.250

(preferably .gtoreq.500). Boron may be complexed with a saccharide having co-planar cis-OH groups capable of forming five or six membered rings through ester bonding with boric acid. The complexes can include fructose, mannose, or sorbose. Alternatively, a carbohydrate-boric acid complex may be charge neutralized with calcium, magnesium or other cations. Thus, boric acid is added to a soln. of D-fructose, and calcium carbonate is added to produce calcium **fructoborate**. The boron supplement can be included in a food, esp. in a high-magnesium food, and particularly a snack food contg. chocolate and(or) nuts.

REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L2 ANSWER 4 OF 4 CAPLUS COPYRIGHT 2004 ACS on STN

ACCESSION NUMBER: 1922:17911 CAPLUS
DOCUMENT NUMBER: 16:17911
ORIGINAL REFERENCE NO.: 16:3070f-i
TITLE: Constitution and rotatory powers of mannitol and fructose complexes formed in solutions containing boric acid and sodium hydroxide
AUTHOR(S): van Barneveld Gilmour, George
SOURCE: Journal of the Chemical Society, Abstracts (1922), 121, 1333-40
CODEN: JCSAAZ; ISSN: 0590-9791
DOCUMENT TYPE: Journal
LANGUAGE: Unavailable

AB Rotation measurements have been made with the view of showing the effects of reagents on mannitoboric acid (A) and fructoboric acid (B) or their salts rather than on the alc. and sugar. In the case of A the rate of increase in rotation is roughly proportional to the NaOH added until about 1/3 of the equiv. is present, beyond which the increase is still proportional but greater than the rate during the earlier stage. Addition in excess of the equiv. is practically without effect. The rate of decrease in the case of B is proportional to the NaOH added until about 1/3 equiv. is present and then it falls off with each addn. This indicates that in solns. of acids like A the mols. are associated in groups of 3, probably having an oxonium structure. The change that takes place after about 1/3 equiv. has been added is possibly due to the breaking up of the complex. mols. In the case of solns. containing 2 mols. mannitol to 1 of A, or of fructose and B, the rate of change in rotation in both cases is approx. proportional to the NaOH added until 1 equiv. is present. When the equiv. of NaOH is present, the complexes trimannitol-NaBO2 and trifructose-NaBO2 must be present. From the regularity in the rate of change in rotation, the complexes are probably formed before the addition of the alkali. The addition of H3BO3 lowers the rotation of Na mannitoborate (C) and raises that of Na **fructoborate** (D) while the opposite effect is obtained with NaBO2. The rotation of mannitol in the form of C was found to be [.alpha.]D 22.1.degree., that of fructose in the form of D [.alpha.]D -35.2.degree.. Concn. seems to affect the rotation of C and D very little.